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Superconductivity and Electronic Structure of the $W_7Re_{13}B$ Compound

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The superconductor $W_7Re_{13}B$ has been studied by the magnetic measurements and microwave absorption. The crystal structure of $W_7Re_{13}B$ is cubic (β-Mn type). This compound exhibits a sharp superconducting transition at a temperature of $T_c = 7.2$ K. The electronic structure of $W_7Re_{13}B$ has been studied by X-ray photoelectron spectroscopy and the band structure has been calculated by the full-potential local-orbital minimum-basis method using the scalar-relativistic mode. The main contribution to the density of states at the Fermi level is from $5d$ electrons of W and Re. The W and Re bands are similar and substituting W by Re does not change the total density of states.

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1. Introduction

Superconductivity in $W_7Re_{13}X$ (X = B, C) was discovered by Kawashima et al. [1] in 2004. However, the structural properties of this material were established already in 1968 by Kuz'ma et al. [2]. The crystal structure of $W_7Re_{13}B$ is cubic (β-Mn type, space group $P4_132$) with the $8(c)$ and $12(d)$ sites occupied by W and Re atoms, respectively [3]. This structure is stabilized by the small B content in the vacant space. Based on the temperature dependence of the electron specific heat below T_c the symmetry of superconductivity was established to be isotropic s-wave [1]. The lower and the upper critical fields were found to be $H_{c1}(0) = 77$ Oe and $H_{c2}(0) = 114$ kOe and the correlation length was equal to 54 Å.

In this paper we present the magnetic and electronic structure studies of $W_7Re_{13}B$ by magnetic measurements, X-ray photoemission spectroscopy (XPS), and theoretical calculations.

2. Results and discussion

The $W_7Re_{13}B$ compound was prepared by induction melting of the constituent elements in a water-cooled boat, under an argon atmosphere. The crystallographic structure was established by X-ray diffraction technique. The determined lattice constant, equal to 6.820 Å, is in good agreement with the previous studies [1].

The magnetic measurements were carried out by means of the magnetometer MagLab 2000 System (Oxford Instruments Ltd.).

The measurements of the magnetically modulated microwave absorption (MMMA) were performed using a commercial X-band (9.4 GHz) EPR spectrometer (SE/X Radiopan Ltd.) equipped with an ESR 900 helium-flow Oxford Instruments Ltd. Cryostat.

The X-ray photoemission spectra were obtained for the radiation of the photon energy equal to 1487.6 eV (Al K_α source) using a PHI 5700/660 Physical Electronics Spectrometer. All emission spectra were measured immediately after breaking the sample in a vacuum of 10^{-10} Torr.

The electronic structure was calculated for the ordered W_8Re_{14} compound (space group $P4_132$) and the lattice constant $a = 6.819$ Å. The positions of the atoms are: W (0.061, 0.061, 0.061) and Re (1/8, 0.206, 0.486). The unit cell consisted of 20 atoms. We used the full-potential local-orbital minimum-basis code (FPLO) and the band structure was calculated in the scalar-relativistic mode [4]. In the FPLO scheme the calculations were performed using the full potential local orbital minimum basis. The parameterization of the exchange-correlation potential in the framework of the local spin density approximation was used in the form proposed by Perdew [5].

Figure 1 presents the zero field cooling magnetization of the $W_7Re_{13}B$ superconductor in an applied magnetic field of 10 Oe. This compound exhibits a sharp superconducting transition at a temperature of $T_c = 7.2$ K with the transition width at 50% of diamagnetic signal equal to $T_c(50\%) = 0.2$ K. One degree below the transition, the diamagnetic signal saturates and does not change with the further temperature decrease.

Figure 2 shows the MMMA signal recorded for the same sample in zero applied magnetic field. The microwave absorption appears at the critical temperature of $T_c = 6.8$ K and then exhibits a sharp peak associated with the superconducting transition. The width of the peak measured at 50% of the MMMA signal is, like in the magnetometric studies, equal to 0.2 K. The microwave absorption in lower temperatures is very small. The sharp transition observed both in the magnetic and microwave measurements proves that the sample is homogeneous and contains no internal weak links or Josephson junctions. The inset of Fig. 2 displays an example of the MMMA loop.

The minor hysteresis loop recorded at a temperature of $T = 2$ K and in the magnetic field range ±100 Oe is open, which proves that magnetic flux penetrates

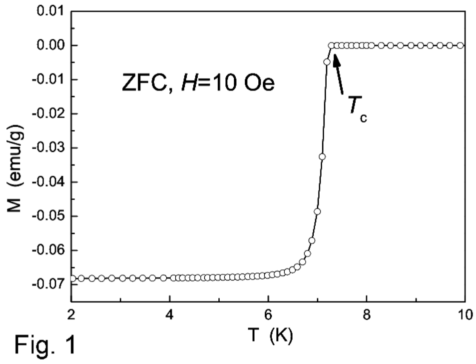

Fig. 1

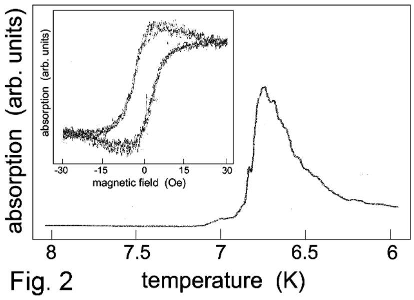

Fig. 2

Fig. 1. Zero-field cooling curve indicating the transition to superconductivity at 7.2 K for the $W_7Re_{13}B$ compound.

Fig. 2. MMMA as a function of temperature. Inset: MMMA loop measured at 5.7 K.

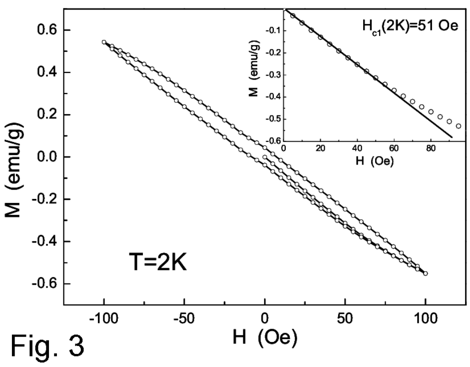

Fig. 3

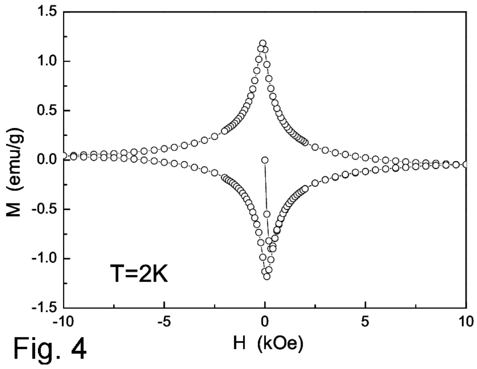

Fig. 4

Fig. 3. Minor hysteresis loop recorded at 2 K. Inset: determination of $H_{c1}(T)$.

Fig. 4. Major hysteresis loop recorded at a temperature of $T = 2$ K.

the sample (Fig. 3). The magnetic flux enters the sample when the magnetization $M(H)$ starts to deviate from a linear behavior. From the inset of Fig. 3 it is visible that it occurs for $H = 50$ Oe. Using the parabolic relation for the lower critical field dependence on temperature, $H_{c1}(T) = H_{c1}(0)[1 - (T/T_c)^2]$, one obtains $H_{c1}(0) \approx$ 54 Oe. The high value of the $M(H)$ slope proves that the $W_7Re_{13}B$ compound is a "bulk" superconductor.

The major hysteresis loop, recorded at the same temperature as the minor one and at the field range of ± 10 kOe is shown in Fig. 4. The width of the loop decreases rapidly as the magnetic field increases. This behavior indicates that the critical current is also strongly field dependent and that the flux pinning in the superconductor is rather weak.

Figure 5a shows the valence-band XPS spectrum of $W_7Re_{13}B$. Based on the FPLO calculations plotted as the total density of states (DOS) in Fig. 5b, it results that the main contribution in the binding energy range –7–0 eV comes from the

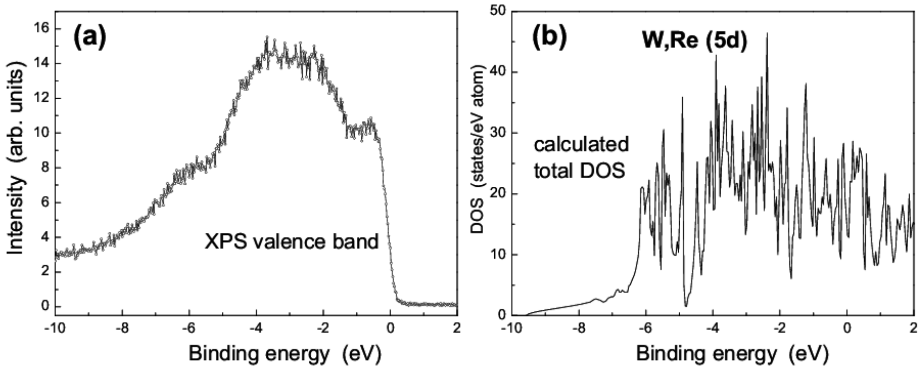

Fig. 5. The XPS valence band spectrum of $W_7Re_{13}B$ (a) and the FPLO calculation of the total DOS (b).

W(5d) and Re(5d) states. The W and Re bands are similar, therefore the partial DOS of them is not displayed. The prominent features in the XPS valence band region are due to the multiplet effects. The density of states at the Fermi level is $N(E_F) = 431$ states/Ry.

3. Conclusions

The transition of the $W_7Re_{13}B$ compound to the superconducting state was observed both in the magnetometric studies and microwave absorption measurements at about 7.2 K. In both cases the transition is very sharp with the width of about 0.2 K. The MMMA results suggest the absence of any internal weak links or Josephson junctions. The lower critical field is $H_{c1}(0) \approx 54$ Oe.

The X-ray photoemission studies supported by the FPLO calculations show that the binding energy range from −7 eV to the Fermi level (0 eV) is dominated by the W and Re 5d states. The partial DOS of the two elements is very similar.

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